Electronic Supplementary Information

for

A folding decalin tetra-urea for transmembrane anion transport

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1. NMR spectra of amine **8**

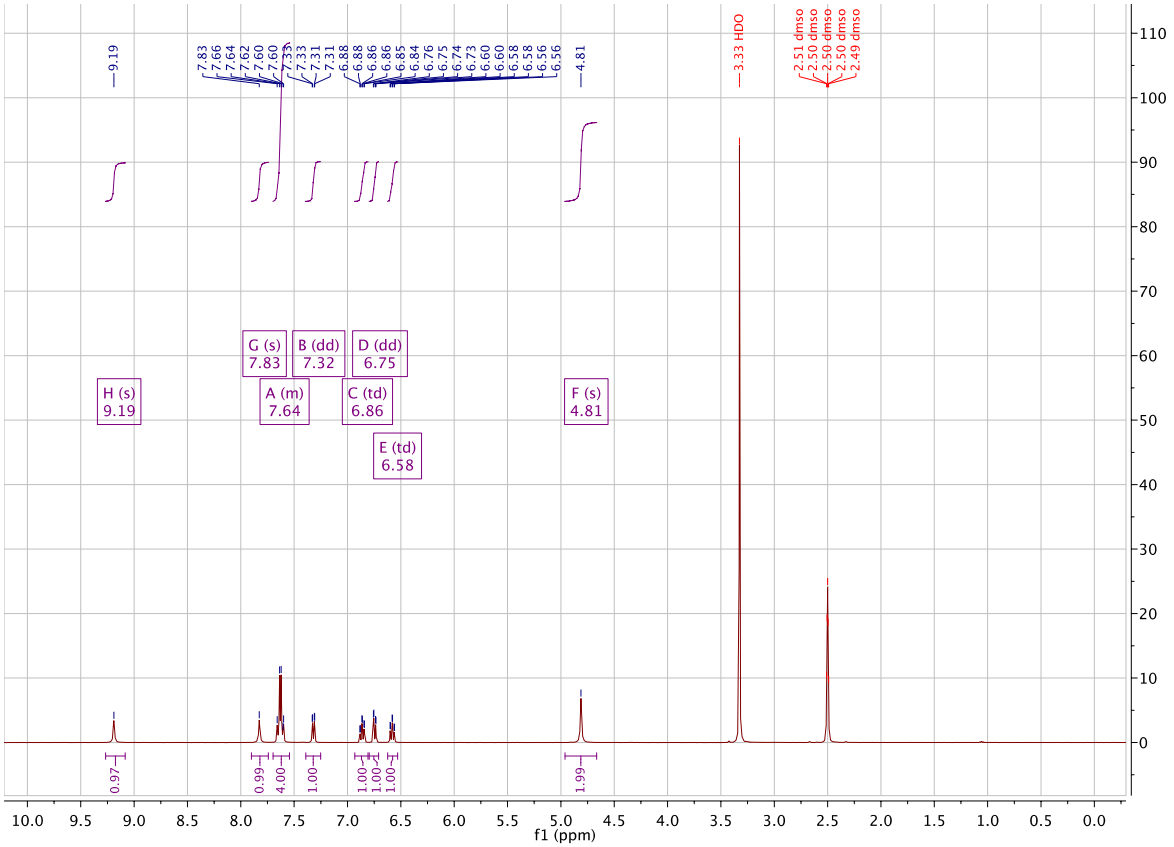


Figure S1. ^{1}H NMR spectrum of amine **8** in DMSO-d_6 (400 MHz).

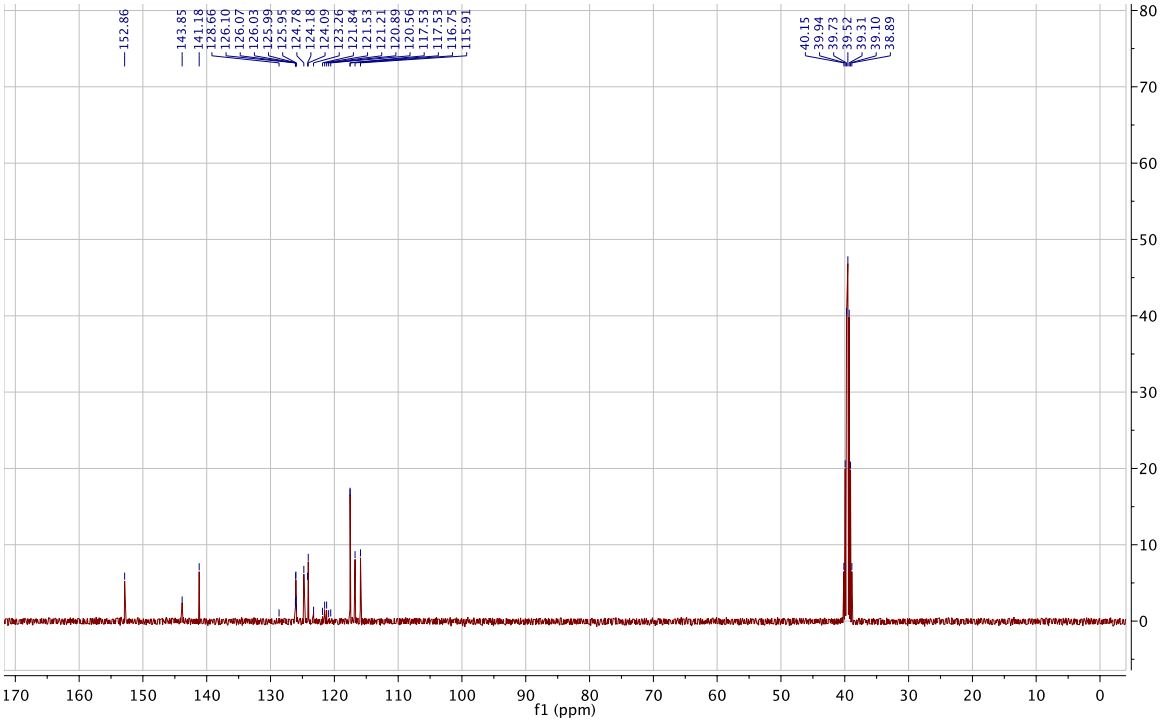


Figure S2. ^{13}C NMR spectrum of amine **8** in DMSO-d_6 (101 MHz).

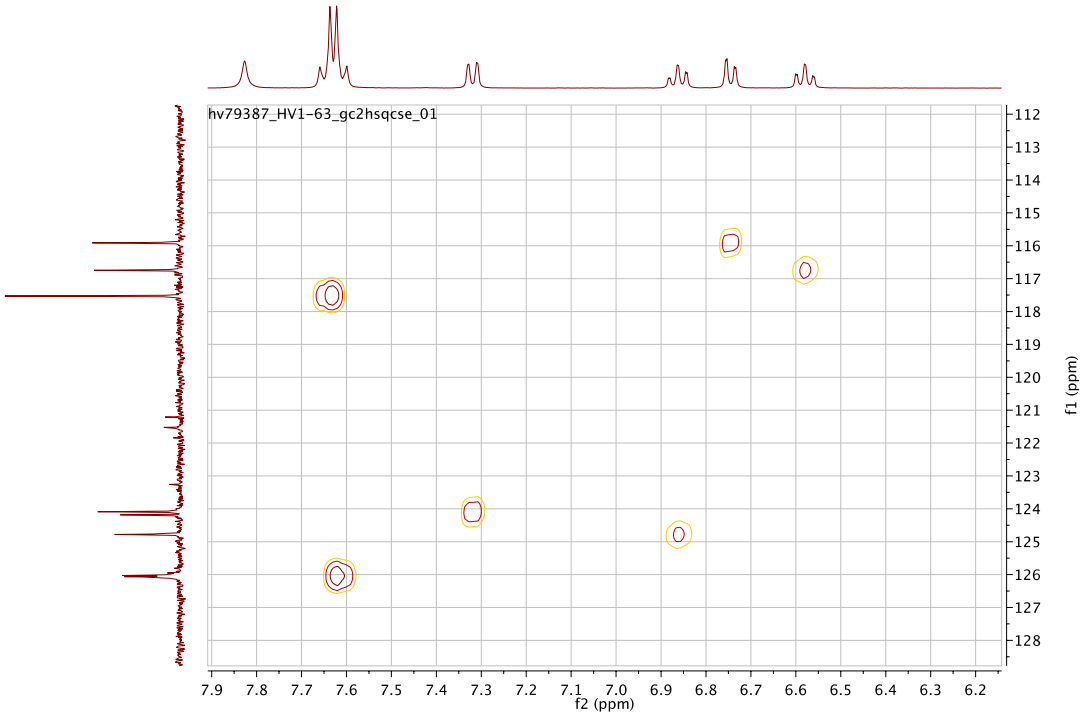


Figure S3. HSQC spectrum of amine **8** in DMSO-d_6 (400 MHz).

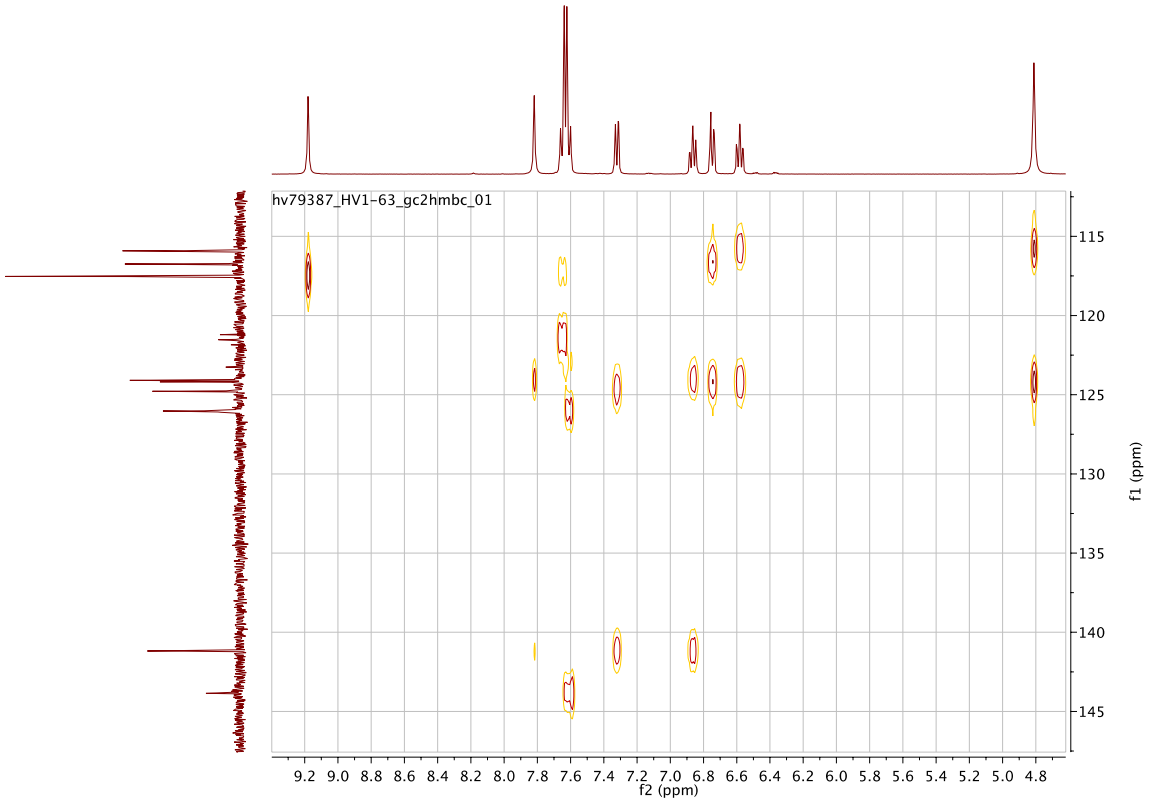


Figure S4. HMBC spectrum of amine **8** in DMSO-d_6 (400 MHz).

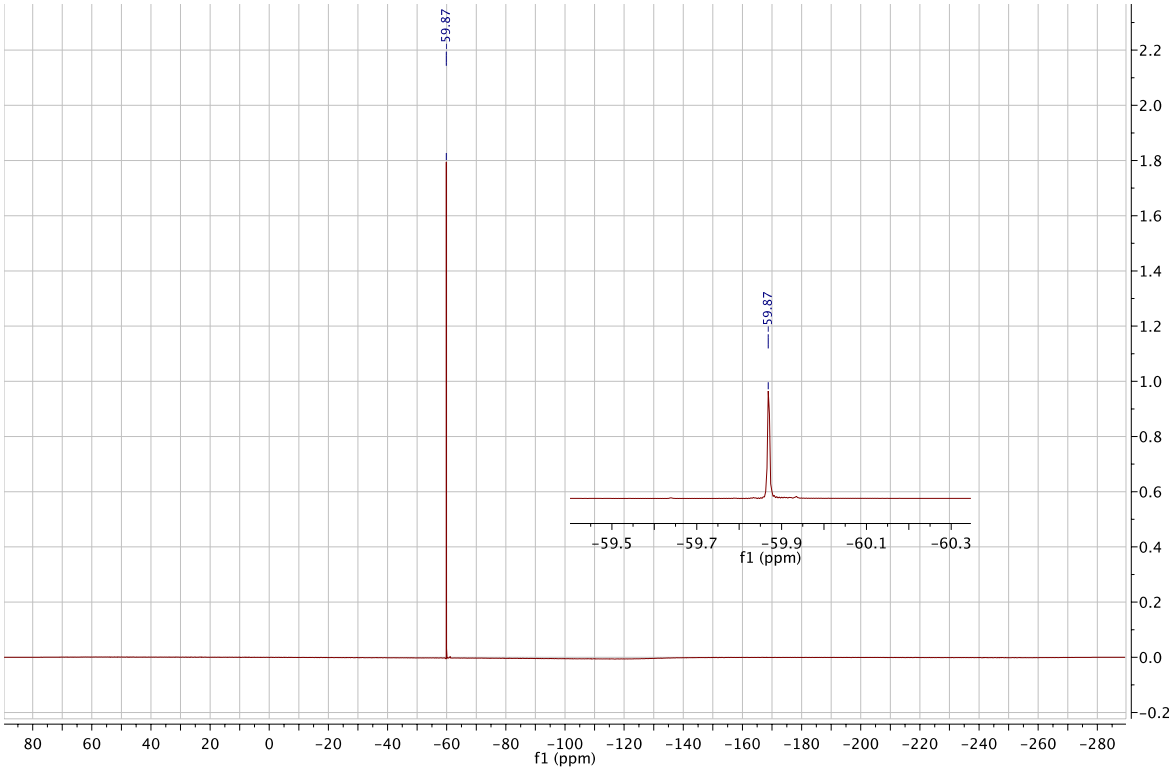


Figure S5. ^{19}F spectrum of amine **8** in DMSO-d_6 (377 MHz).

2. NMR spectra of decalin tetra-urea **7**

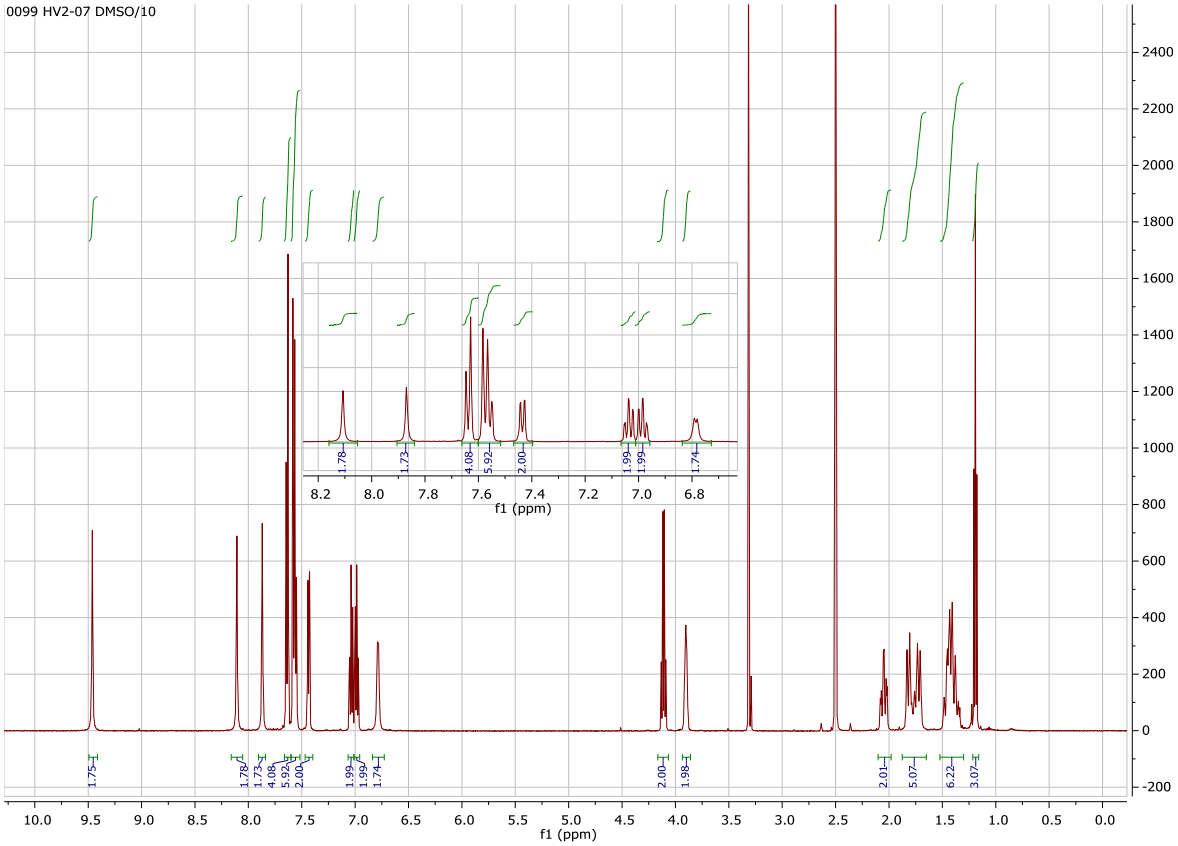


Figure S6. ^{1}H NMR spectrum of **7** in DMSO-d_6 (500 MHz).

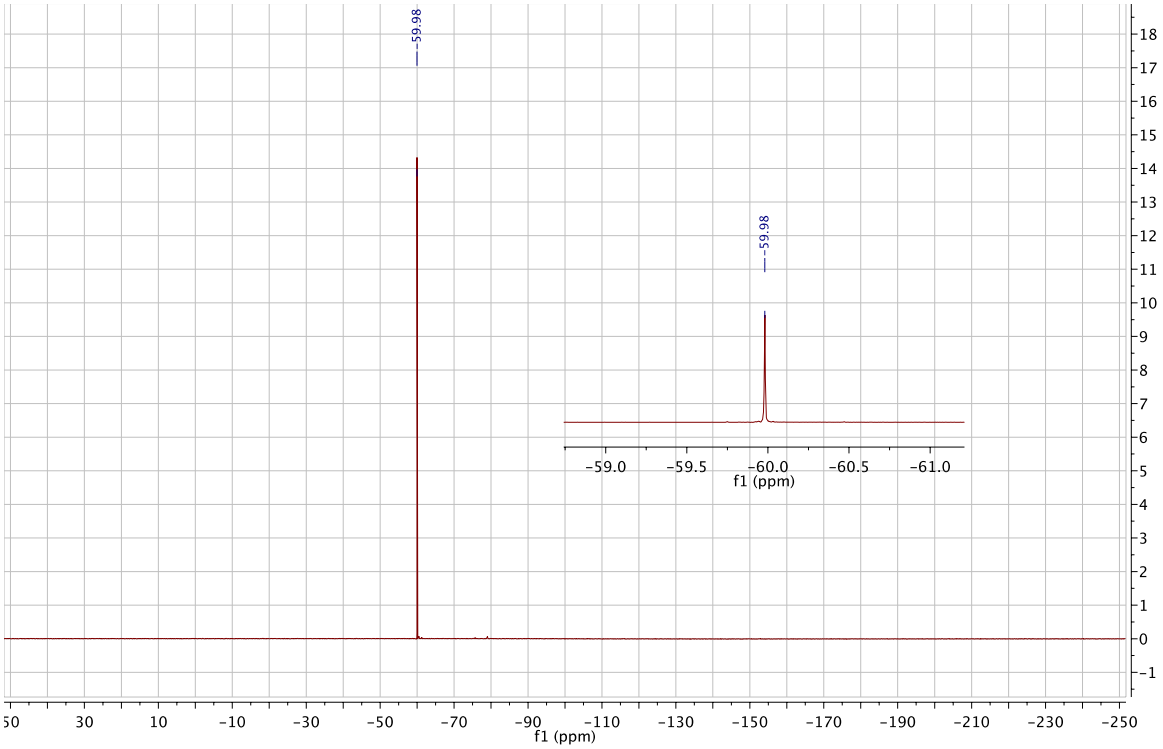


Figure S7. ^{19}F spectrum of **7** in DMSO-d_6 (377 MHz).

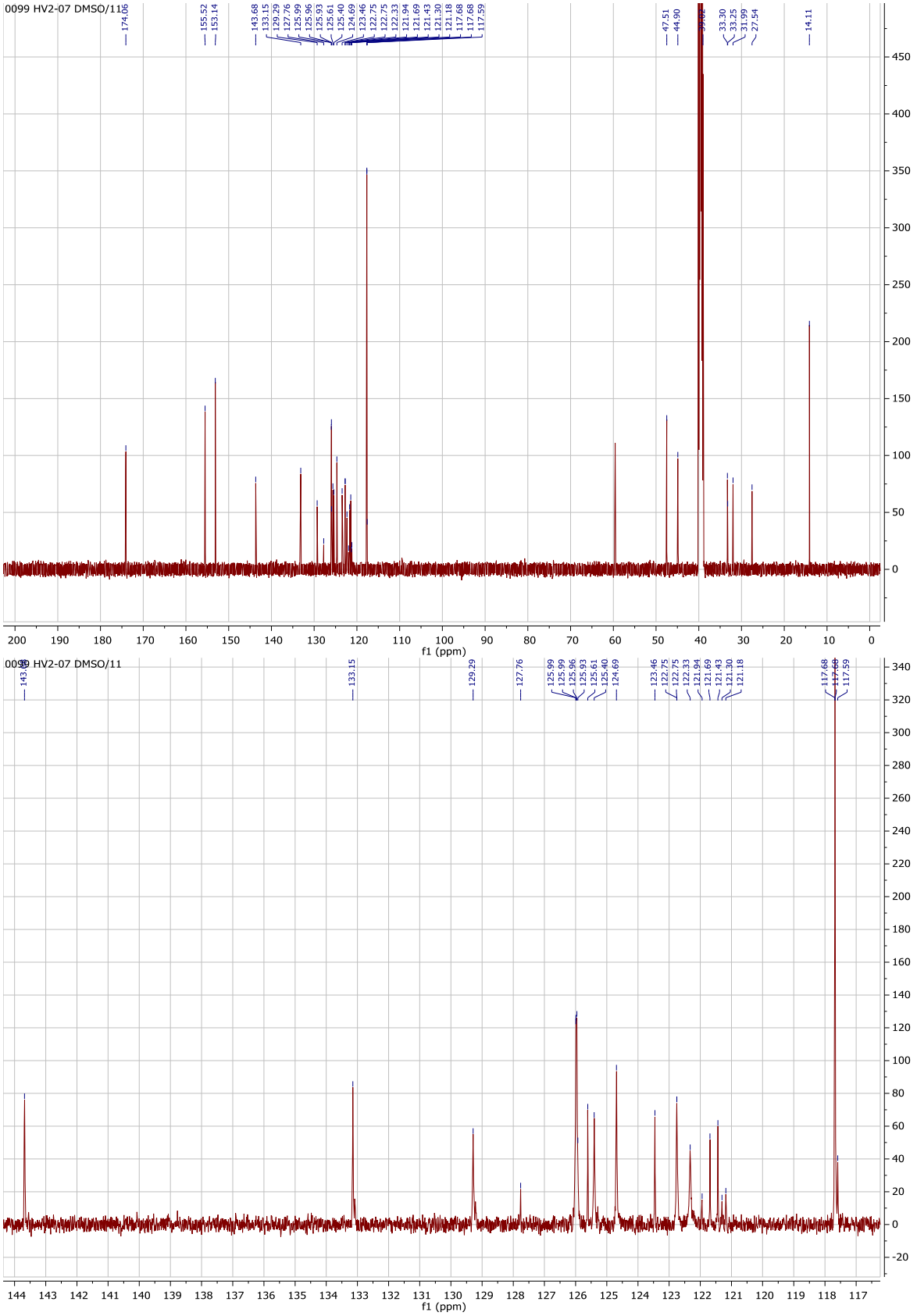


Figure S8. ^{13}C NMR spectra of **7** in DMSO-d_6 (126 MHz).

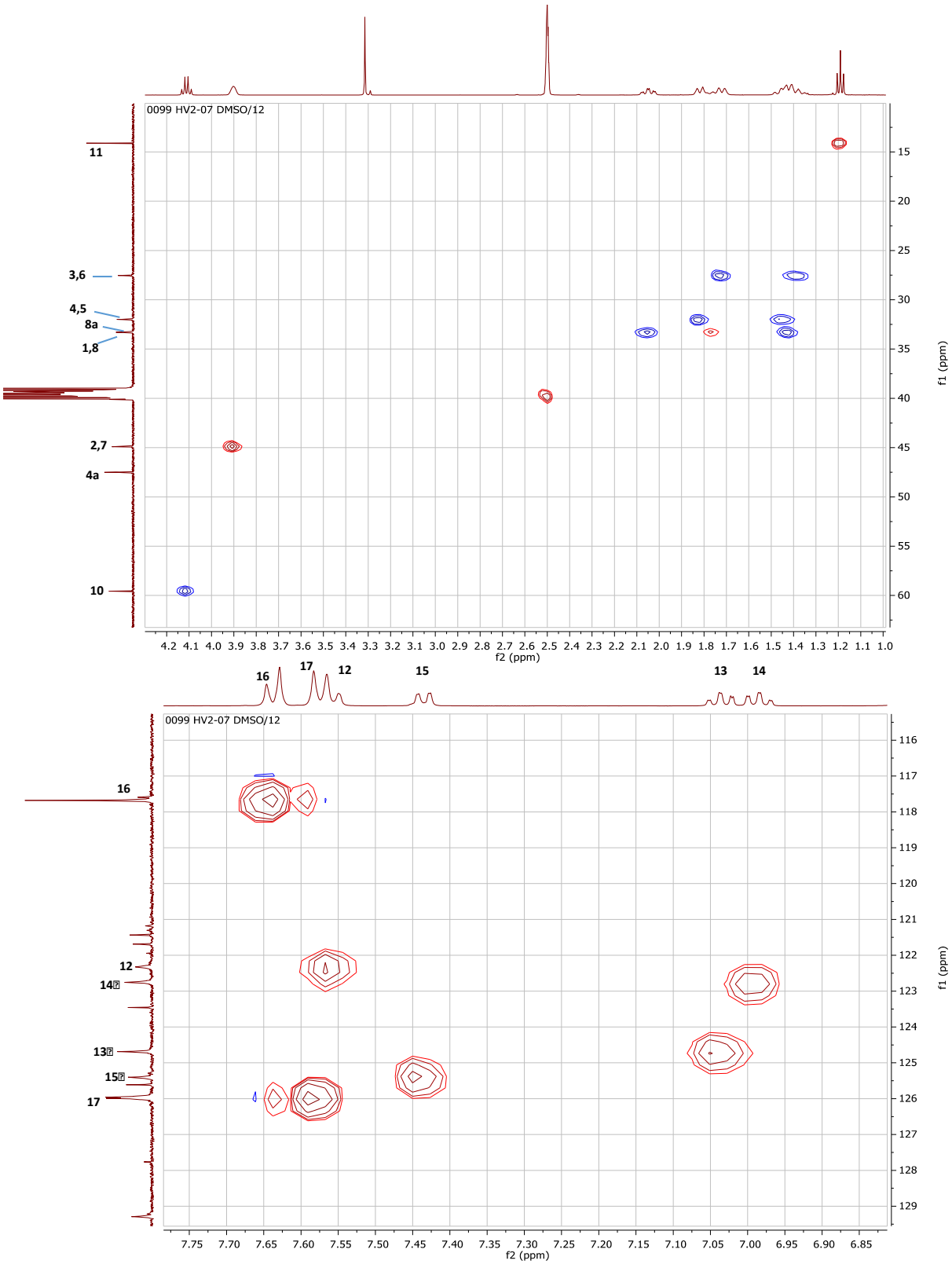


Figure S9. HSQC spectra of **7** in DMSO-d_6 (500 MHz).

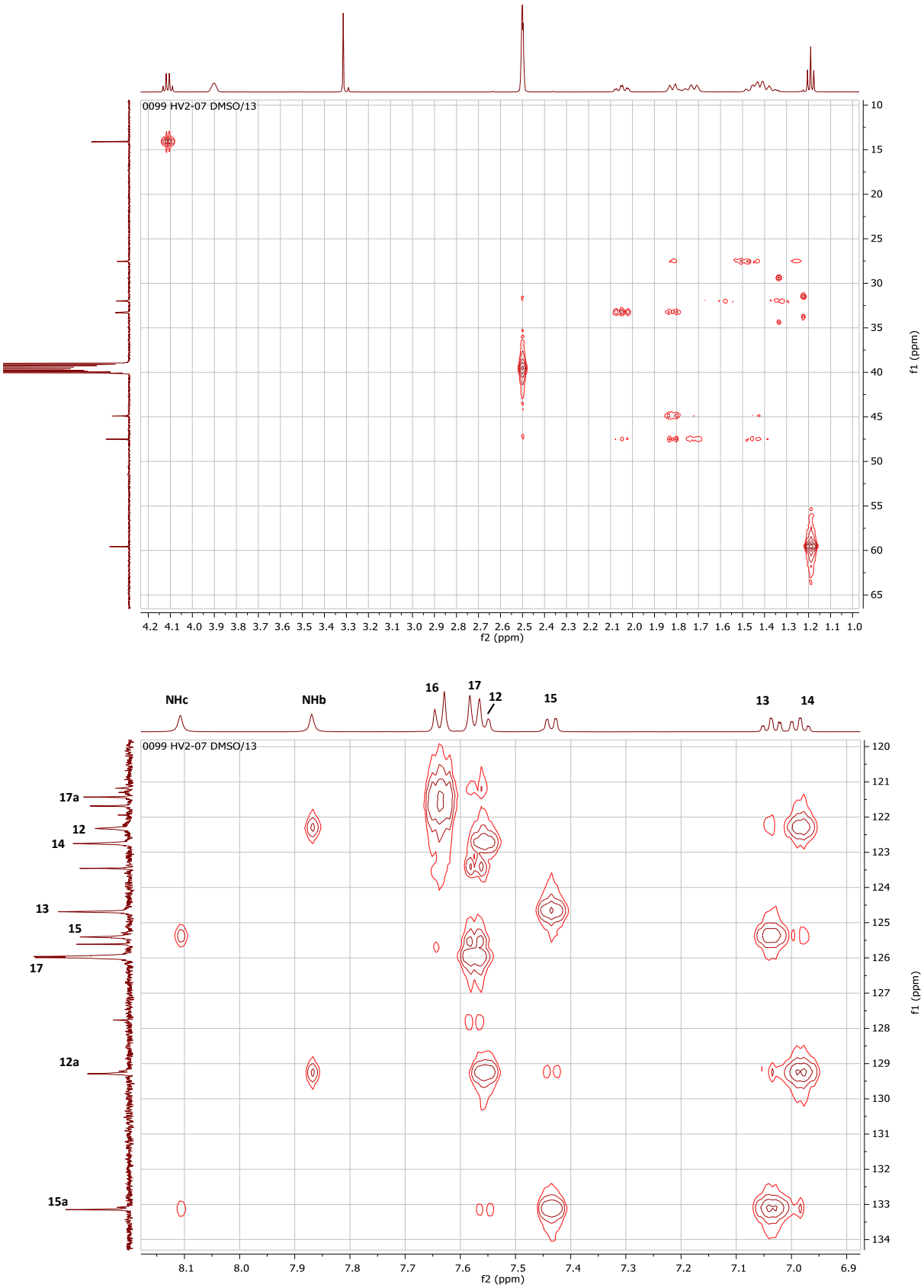


Figure S10. HMBC spectra of **7** in DMSO-d_6 (500 MHz).

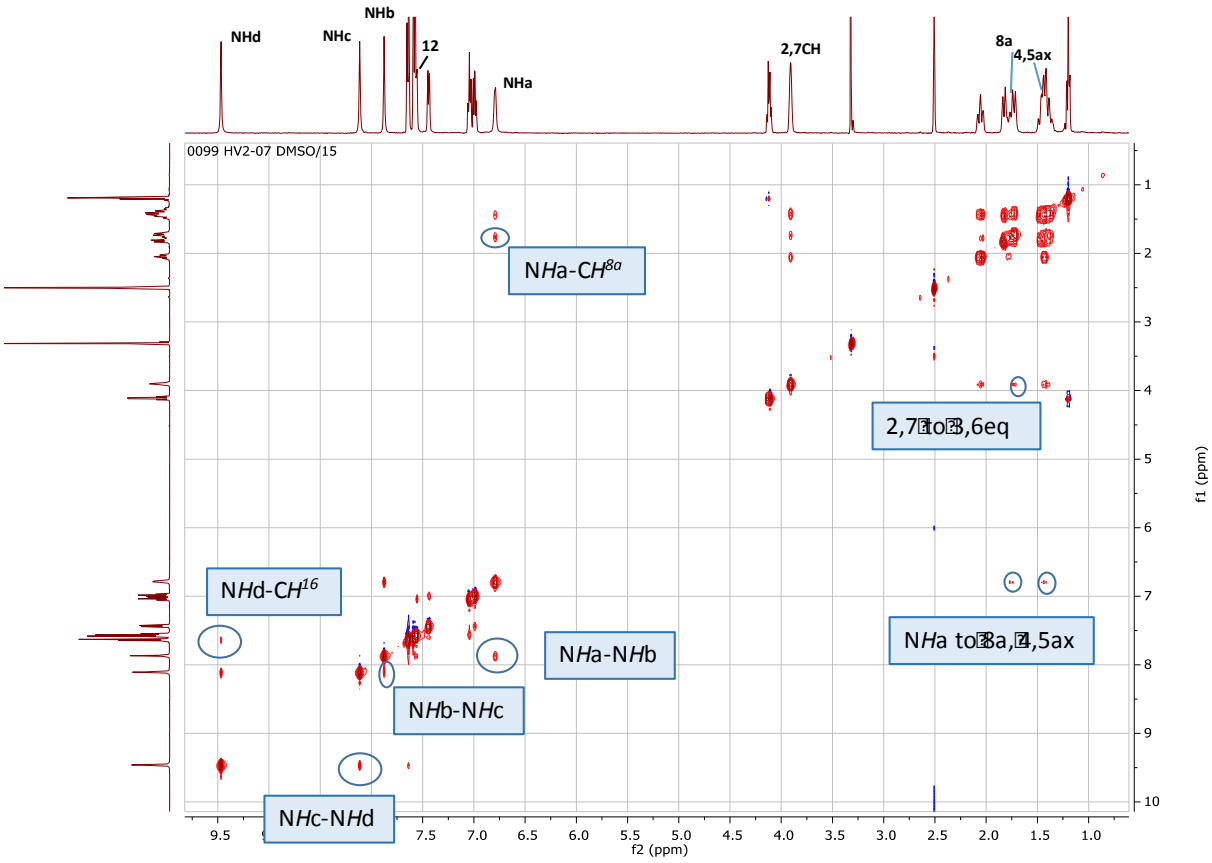


Figure S11. 2D NOESY spectrum of **7** in DMSO-d_6 (500 MHz).

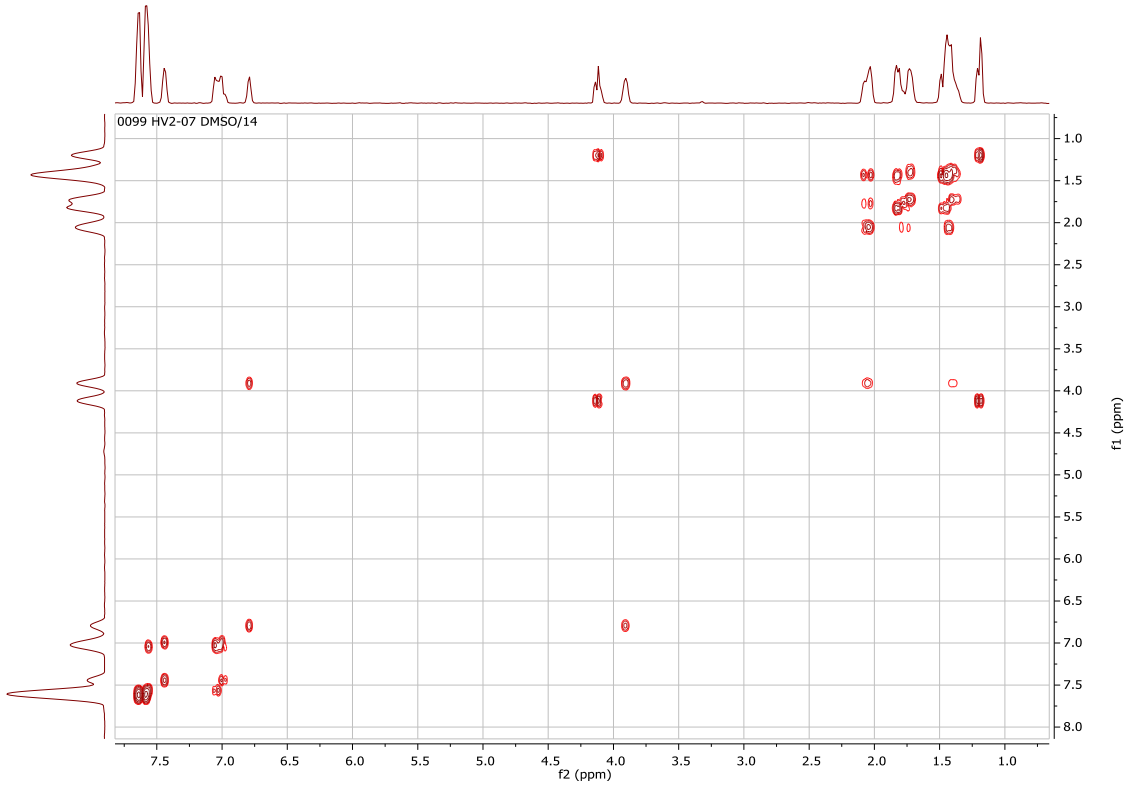


Figure S12. 2D COSY spectrum of **7** in DMSO-d_6 (500 MHz).

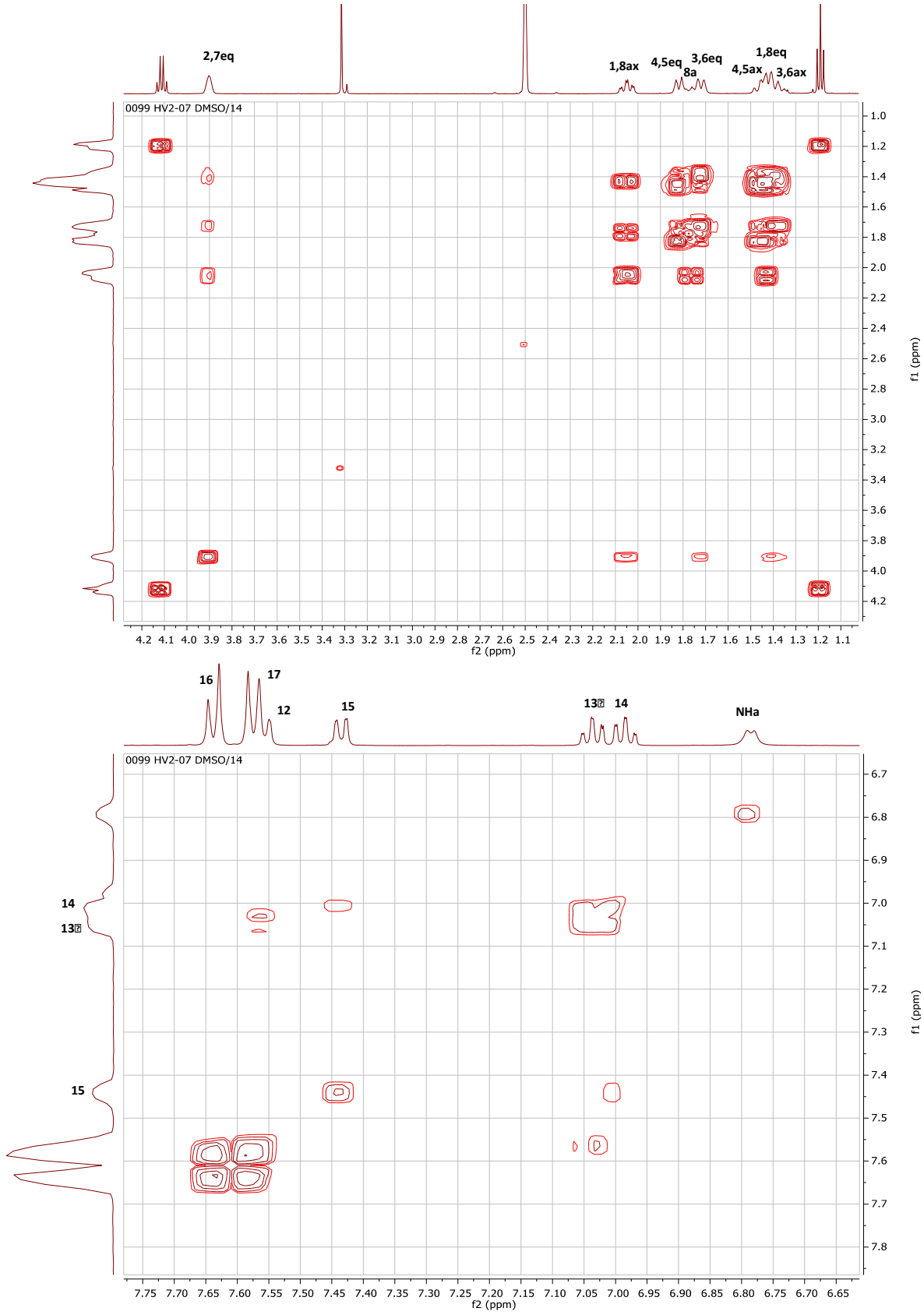


Figure S13. 2D COSY spectra of **7** in DMSO-d_6 (500 MHz).

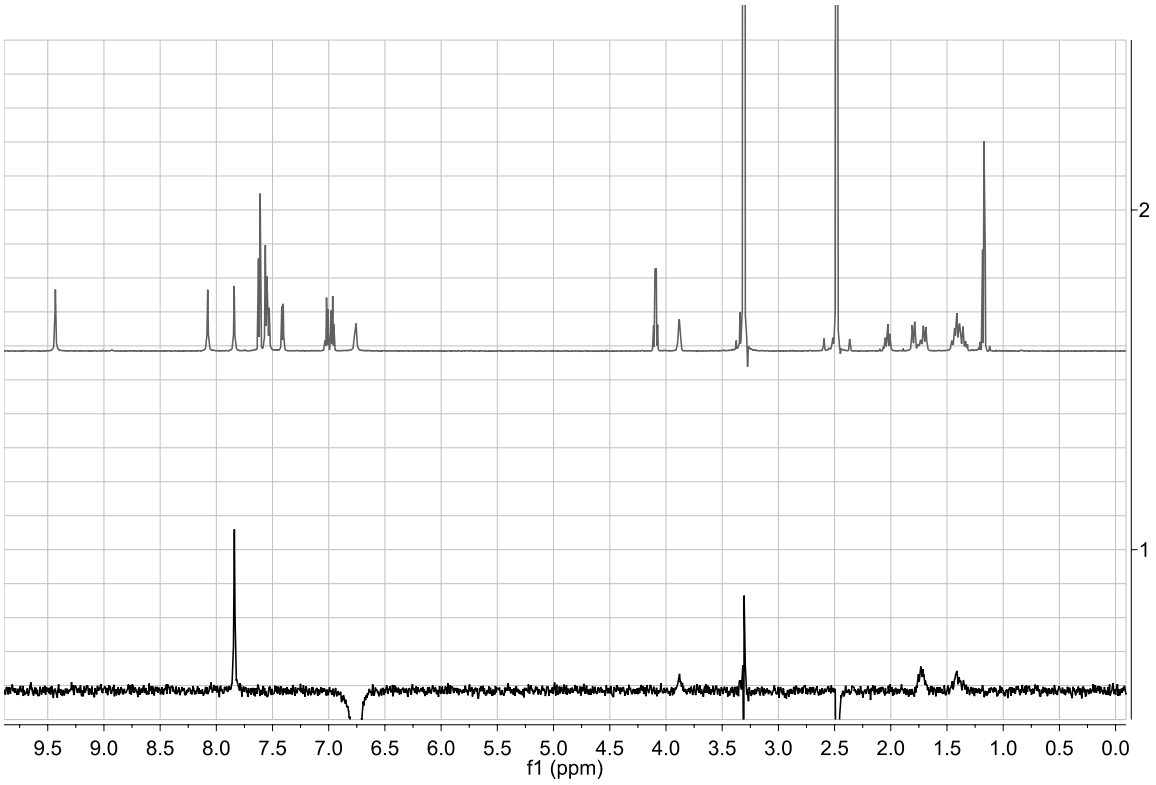


Figure S14. ^{1}H NMR spectrum of **7** in DMSO-d_6 (top; 600 MHz) and 1D ROESY spectrum of **7** in DMSO-d_6 with N*H*^{a} inverted (bottom; 600 MHz).

3. Additional anion transport data and graphs

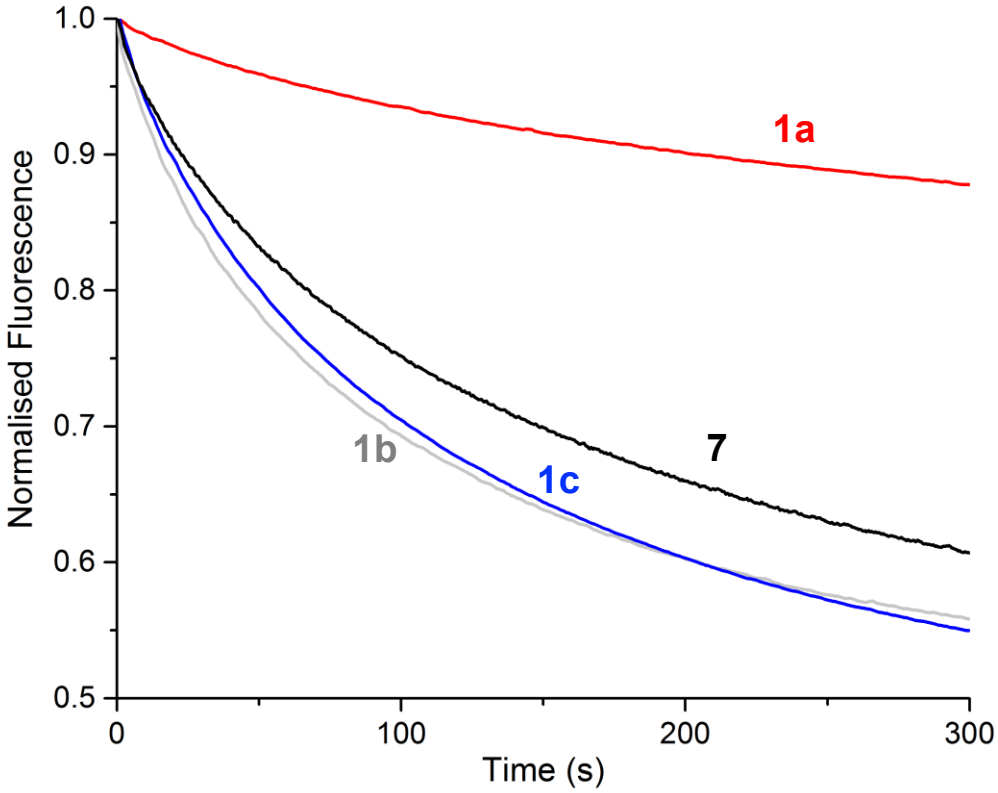
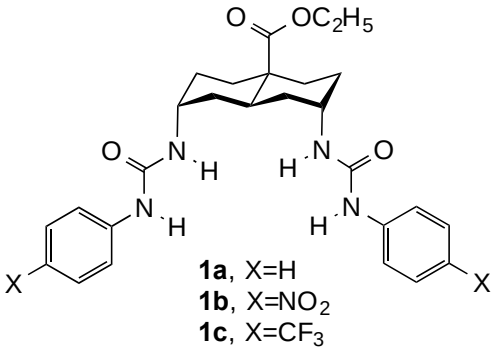
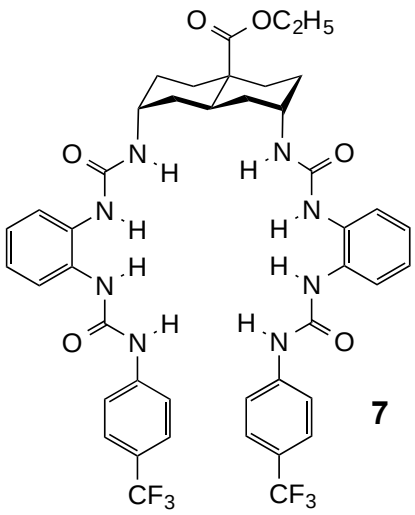


Figure S15. Comparison of the rates of anion transport by **7** with that of previously reported compounds **1a**-**c**.[1,2] All compounds were preincorporated at a transporter to lipid ratio of 1:2500 in liposomes composed of POPC and cholesterol (7:3, 0.4 mM total lipid concentration), containing lucigenin. $NaNO_3$ (225 mM) was present both inside and outside of the liposomes and the transport measurement was initiated by addition of a pulse of NaCl (25 mM).





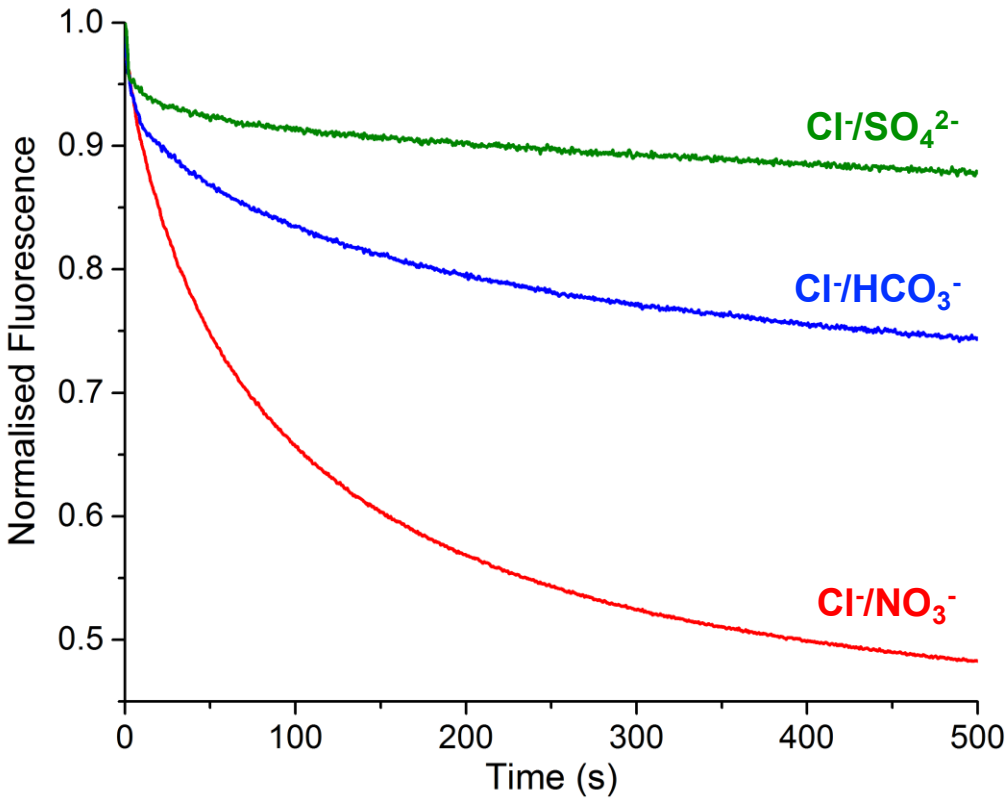


Figure S16. Comparison of the rates of anion transport by **7** in the presence of different anions. Carrier **7** was preincorporated at a transporter to lipid ratio of 1:1000 in liposomes composed of POPC and cholesterol (7:3), containing lucigenin. Either $NaNO_3$ (225 mM), or $NaHCO_3$ (225 mM) or K_2SO_4 (225 mM) was present both inside and outside of the liposomes. The observed trends are similar as those previously found for decalin bis-ureas.[1,3]

References

[1] Hussain S, Brotherhood PR, Judd LW, Davis AP. *J Am Chem Soc* 2011;133:1614.
[2] Li H, Valkenier H, Judd LW, Brotherhood PR, Hussain S, Cooper JA, et al. *Nat Chem* 2016;8:24.
[3] Lisbjerg M, Valkenier H, Jessen BM, Al-Kerdi H, Davis AP, Pittelkow M. *J Am Chem Soc* 2015;137:4948.